DIFFERENTIAL SENSITIVITY THEORY APPLIED TO THE MESA2D CODE FOR MULTI-MATERIAL PROBLEMS

R. J. Henninger, P. J. Maudlin, and E. N. Harstad

Los Alamos National Laboratory, Los Alamos, New Mexico 87545

The technique called Differential Sensitivity Theory (DST) is extended to the multi-component system of equations solved by the MESA2D hydrocode. DST uses adjoint techniques to determine exact sensitivity derivatives, i.e., if R is a calculation result of interest (response R) and α_i is a calculation input (parameter α_i), then $\partial R/\partial \alpha_i$ is defined as the sensitivity. The advantage of using DST is that for an n-parameter problem *all* n sensitivities can be obtained by integrating the solutions from only *two* calculations, a MESA calculation and its corresponding adjoint calculation using an Adjoint Continuum Mechanics (ACM) code. Previous papers have described application of the technique to one-dimensional, single-material problems. This work presents the derivation and solution of the additional adjoint equations for the purpose of computing sensitivities for two-dimensional, multi-component problems. As an example, results for a multi-material flyer plate impact problem featuring an oblique impact are given.

INTRODUCTION

A sensitivity technique (1-3) used successfully in the early eighties (4-6) called Differential Sensitivity Theory (DST) is applied to a system of time-dependent continuum mechanics equations (7). DST uses adjoint techniques to determine exact sensitivity derivatives, i.e., if R is a calculational result of interest (response R) and α is a calculational input (parameter α_i where the subscript is usually not indicated for convenience), then $\partial R/\partial \alpha_i$ is defined as the sensitivity. The advantage of using DST over other sensitivity analysis techniques is mainly economic: for an n-parameter problem *all* n sensitivities can be obtained by integrating the solutions from only *two* calculations, a so-called forward (physical) calculation and its corresponding adjoint calculation. This work describes the derivation and solution of the appropriate set of adjoint and sensitivity equations for the ultimate purpose of computing sensitivities for high-rate two-dimensional, multi-component, high deformation problems.

Following Cacuci et. al. (2), consider a system of nonlinear equations written in symbolic form as

$$N\left[\bar{y}(\bar{x}), \bar{\alpha}\right] = O(\bar{x}, \bar{\alpha}) , \qquad (1)$$

where $\bar{y}$ is a dependent variable vector, $\bar{x}$ is an independent variable vector and $\bar{\alpha}$ is a parameter vector. Also we assume a response function having the general form:

$$R = \int_t \int_{\bar{r}} F(\bar{y}, \bar{x})\, d\bar{r}\, dt \equiv \left\langle F(\bar{y}, \bar{x}) \right\rangle \qquad (2)$$

where the angle brackets denote space-time integration. If Eq. 1 is differentiated with respect to an arbitrary parameter α, then the resulting system of equations is linear with respect to the new differentiated dependent variable vector, and has the form:

$$\mathbf{L} \frac{\partial \bar{y}}{\partial \alpha} = \bar{s} , \qquad (3)$$

where $\mathbf{L}$ is a linear operator operating on the dependent variable vector and $\bar{s}$ represents a vector source term that contains the problem parameters differentiated with respect to α. Taking the partial with respect to α of the response (Eq. 2) gives

$$\frac{\partial R}{\partial \alpha} = \int_t \int_{\vec{r}} \frac{\partial F}{\partial \vec{y}} \bullet \frac{\partial \vec{y}}{\partial \alpha} d\vec{r} dt \equiv \left\langle \frac{\partial F}{\partial \vec{y}}, \frac{\partial \vec{y}}{\partial \alpha} \right\rangle \tag{4}$$

Taking the inner product of the left-hand side of Eq. 3 with an arbitrary vector function $\vec{y}^*$ and invoking a property of inner-product spaces gives

$$\left\langle \vec{y}^{*}, \mathbf{L} \frac{\partial \vec{y}}{\partial \alpha} \right\rangle = \left\langle \frac{\partial \vec{y}}{\partial \alpha}, \mathbf{L}^{*} \vec{y}^{*} \right\rangle + B\left(\vec{y}^{*}, \frac{\partial \vec{y}}{\partial \alpha} \right), \tag{5}$$

where the function B represents the appropriate boundary terms. This equation can be used to derive a linear adjoint to $\mathbf{L}$ (i.e., $\mathbf{L}^*$) that operates on $\vec{y}^*$ and, when set equal to the differentiated response function from the integrand of Eq. 4, this system of equations can be solved for the so-called adjoint solution:

$$\mathbf{L}^{*} \vec{y}^{*} = \frac{\partial F}{\partial \vec{y}} \tag{6}$$

Substituting Eq. 6 into the right-hand side of Eq. 4, using the inner product property given by Eq. 5, and substituting again with Eq. 3 gives

$$\frac{\partial R}{\partial \alpha} = \left\langle \mathbf{L}^{*} \vec{y}^{*}, \frac{\partial \vec{y}}{\partial \alpha} \right\rangle = \left\langle \vec{y}^{*}, \vec{s} \right\rangle - B\left(\vec{y}^{*}, \frac{\partial \vec{y}}{\partial \alpha} \right) \tag{7}$$

The last right-hand-side of this equation represents the final integral form of the sensitivity $\partial R / \partial \alpha$.

Practical application of DST requires the solution of the adjoint system represented by Eq. 6 and the sensitivity integration represented by Eq. 7. In our previous paper (8), we presented the forward equations , showed the adjoint equation set, and provided an example for a single material problem. In what follows, we show the additional terms and equations required for multiple material problems and develop the adjoint equations, whose solution results in the sensitivity of the response to initial material interface position. We then show results for a multi-material flyer in an oblique impact situation.

DST WITH INTERFACES

Material interfaces manifest themselves in the equation set as differences in material properties, hence, differences in the equation of state (EOS). In one dimension this results in discontinuous behavior of the pressure. For a material that is between z_ν and $z_{\nu+1}$ the pressure P is given by

$$P = \sum_{\nu=1}^{N} P_\nu \left[u\langle z - z_\nu \rangle - u\langle z - z_{\nu+1} \rangle \right], \tag{8}$$

where u is the unit step function. The "interface equation" for tracking the ν^{th} material boundary, which moves at velocity u_z, becomes

$$\dot{z}_\nu = \int_0^L u_z \delta\langle z - z_\nu \rangle dz \,. \tag{9}$$

This results in a new dependent adjoint variable ζ_ν^* whose time dependence is given by

$$\dot{\zeta}_\nu^* = -\left.\frac{\partial u_z}{\partial z}\right|_{z_\nu} \zeta_\nu^* + \sum_m \frac{\partial P}{\partial \tilde{\alpha}^m} \left(\alpha_{\nu+1}^m - \alpha_\nu^m \right) \Pi^* \Big|_{z_\nu} \tag{10}$$

where Π^* is the adjoint pressure and the $\tilde{\alpha}^m$ are the interface discontinuous EOS parameters

$$\tilde{\alpha}^m = \left[\left(1 - u\langle z - z_\nu \rangle \right) \alpha_\nu^m - u\langle z - z_{\nu+1} \rangle \alpha_{\nu+1}^m \right].$$

The following additional terms are introduced into the adjoint density, axial velocity, and energy equations, respectively:

$$-\sum_{\nu=1}^{N} \frac{\partial P}{\partial \rho} \Pi^{*}\left[u\langle z-z_{\nu}\rangle - u\langle z-z_{\nu+1}\rangle\right] , \quad (11)$$

$$-\sum_{\nu=1}^{N} \zeta_{\nu}^{*}\ \delta\langle z-z_{\nu}\rangle \text{ , and} \quad (12)$$

$$-\sum_{\nu=1}^{N} \frac{\partial P}{\partial i} \Pi^{*}\left[u\langle z-z_{\nu}\rangle - u\langle z-z_{\nu+1}\rangle\right] , \quad (13)$$

where ρ is the density and i is the internal energy. Numerical approximation of the delta-functions appearing in the adjoint equation set was implemented using the method of Peskin (9).

Extension of the interface equations to two dimensions is straight forward, has been implemented, and is demonstrated below with an oblique impact example.

OBLIQUE FLYER EXAMPLE

Consider the impact of the five-material flyer shown in Fig. 1 with a rigid boundary. The materials identified in the figure are represented by Mie-Grueneisen EOSs (10). The flyer has an initial velocity of 500 m/s. Upon impact the plate experiences a right going shock that compresses the materials. Because the interfaces are at an arbitrary angle, the problem is two-dimensional. The flyer is 1.5 cm in length, 0.5 cm in thickness and is divided into 0.25 mm square cells (60 by 20 cells) for the numerical computations. The impact problem was simulated to a final time of 4.0 µs.

The response for this problem was arbitrarily chosen to be the time-averaged pressure, i.e.,

$$R = \int_{t}\int_{\vec{r}} \frac{P}{t_f V}\, d\vec{r}\, dt = \overline{P} \quad (14)$$

so that the adjoint source (appearing in the adjoint pressure equation) for Eq. 6 is

$$s_{\Pi^*} = \frac{1}{t_f V} , \quad (15)$$

where t_f is the final time and V is the flyer volume. The interface is represented as linear segments between the dots shown in Fig. 1.

The interface sensitivities for this impact problem are given in Fig. 2 for the space-time-average pressure (14.872 GPa). The sensitivity for each marker is given by

$$\frac{\partial R}{\partial z_{\nu o}} = \zeta_{\nu}^{*}\Big|_{t=0} \quad (16)$$

Where $z_{\nu o}$ is the initial axial position of the ν^{th} marker. The figure shows the DST sensitivities as hollow dots connected by a solid line, and the "Direct Method" sensitivities $\Delta R/\Delta\alpha$ (a numerical derivative obtained by determining the change in the response as a result of finite perturbations of each initial axial position) are shown as solid dots connected by a dashed line for validation purposes. Constructing the 20 Direct Method sensitivities required 21 forward calculations, as compared to the 2 calculations (i.e., one forward and one adjoint) needed for the 20 DST sensitivities shown.

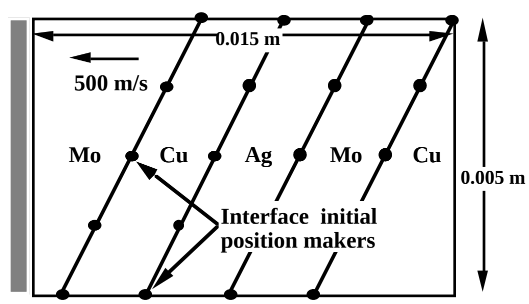

Figure 1. Five-material flyer initial configuration showing interface markers.

SUMMARY AND DISCUSSION

Differential Sensitivity Theory was applied to a two-dimensional set of continuum mechanics equations with a realistic solid phase equation-of-state (i.e., compressible flow) for the purpose of sensitivity analysis. Equations adjoint to a differentiated set of physical equations (differentiated with respect to an arbitrary parameter α) were derived. The resulting DST equation set was illustrated using a two-dimensional flyer impact problem, computing accurate sensitivity coefficients as validated with the Direct Method. Curves comparing DST $\partial R/\partial\alpha$ to Direct Method $\Delta R/\Delta\alpha$ were presented for 20 sensitivities associated with the plate impact problem at a cost of 2 calculations versus 21 calculations, respectively, a saving of 90% in computational time. These low-cost DST sensitivity coefficients can then be used in a subsequent uncertainty analysis, response surface construction or optimization analysis.

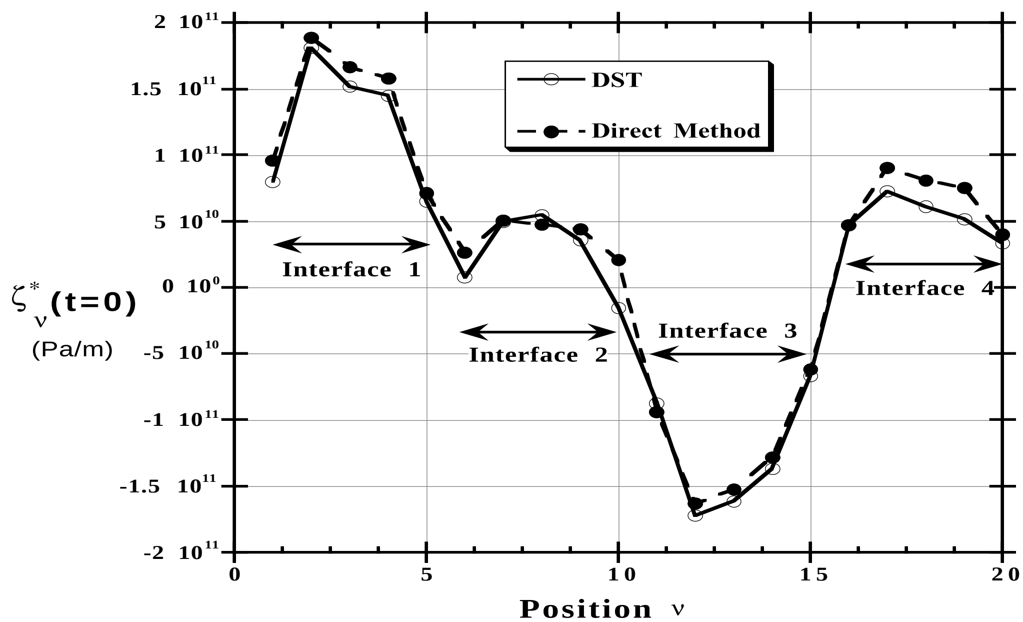

Figure 2. Average pressure sensitivity to initial interface axial position.

REFERENCES

1. E. M. Oblow, "Sensitivity Theory for Reactor Thermal-Hydraulics Problems," *Nucl. Sci. Eng.,* **68**, 322 (1978).
2. D. G. Cacuci, C. F. Weber, E. M. Oblow and J. H. Marable, "Sensitivity Theory for General Systems of Nonlinear Equations," *Nucl. Sci. Eng.*, **75**, 88 (1980).
3. D. G. Cacuci, P. J. Maudlin and C. V. Parks, "Adjoint Sensitivity Analysis of Extremum-Type Responses in Reactor Safety," *Nucl. Sci. Eng.*, **83**, 112 (1983).
4. P. J. Maudlin, C. V. Parks and C. F. Weber, "Thermal-Hydraulic Differential Sensitivity Theory," ASME paper No. 80-WA/HT-56, presented at the ASME Annual Winter Conference (1980).
5. C. V. Parks and P. J. Maudlin, "Application of Differential Sensitivity Theory to a Neutronic/Thermal Hydraulic Reactor Safety Code," *Nucl. Technol.*, **54**, 38 (1981).
6. C. V. Parks, "Adjoint-Based Sensitivity Analysis for Reactor Applications," ORNL/CSD/TM-231, Oak Ridge National Laboratory, 1986.
7. Y. C. Fung, *Foundations of Solid Mechanics*, Prentice-Hall, Inc., Englewood Cliffs, N.J., 1965.
8. R. J. Henninger, P. J. Maudlin, and E. N. Harstad, "Differential Sensitvity Theory Applied to the MESA Code, " Proceedings of the Joint AIRAPT/APS Meeting on High Pressure Science and Technology, page 1781, Colorado Springs, CO (June 28-July 2, 1993).
9. C. S. Peskin, "Numerical Analysis of Blood Flow in the Heart," *J. Comput. Phys.*,25 ,220 ,1977.
10. F. H. Harlow and A. A. Amsden, "Fluid Dynamics," LA-4700, Los Alamos Scientific Laboratory, 1971.